

Few-particle Green's functions for strongly correlated systems on infinite lattices

Mona Berciu

Department of Physics & Astronomy, University of British Columbia, Vancouver, BC, Canada, V6T 1Z1

(Dated: December 9, 2011)

We show how few-particle Green's functions can be calculated efficiently for models with nearest-neighbor hopping, for infinite lattices in any dimension. As an example, for one dimensional spinless fermions with both nearest-neighbor and second nearest-neighbor interactions, we investigate the ground states for up to 5 fermions. This allows us not only to find the stability region of various bound complexes, but also to infer the phase diagram at small but finite concentrations.

PACS numbers: 71.10.Li, 31.15.ac, 71.35.Pq

Recently, there has been considerable interest in few-particle solutions of interacting Hamiltonians. For example, in Ref. [1] it was shown that knowledge of the two- and three-body solutions allows for quantitatively accurate predictions of finite-temperature thermodynamic quantities for many-body systems. As another example, in the context of atomic and molecular physics, the predicted universal three-body Efimov structures [2] have now been seen experimentally [3], giving new impetus to their study and work on various generalizations [4].

While the above work is for free space where particles have parabolic dispersions, there is equally strong interest in the lattice version of such few-body problems. For example, while stable excitons – bound pairs comprised of an electron and a hole – appear in many materials, it is less clear when a so-called charged exciton or trion, consisting of two holes and one electron or viceversa, is stable. That this can happen has been recently demonstrated in GaAs quantum wells [5] and in carbon nanotubes [6]. (Note that trion theory is still mostly based on continuous models and variational solutions, *e.g.* see Ref. [7]). Studying bigger bound complexes, for example bi-exciton pairs, is the next logical step.

Few-particle bound states are relevant not only for the materials where they appear, but also in the interpretation of certain spectroscopic data. For instance, the role played by bound two-particle states, leading to atomic-like multiplet structures in the Auger spectra of narrow-band insulating oxides, is well established [8]. At low dopings, more complicated complexes may form and leave their fingerprints in various spectroscopic features. It is therefore useful to be able to study relatively easily few-particle solutions on an infinite lattice.

In this Letter we show that few-particle Green's functions can be calculated efficiently for strongly correlated lattice Hamiltonians in the thermodynamic limit, at least so long as the hopping involves only nearest neighbor sites. For simplicity and to illustrate the technique and its usefulness, we focus here on a one-dimensional (1D) model of spinless fermions with nearest-neighbor (nn) and next-nearest-neighbor (nnn) interactions. However, the method generalizes straightforwardly to higher dimensions, longer (but finite) range interactions, mixtures

of fermions (including spinful fermions) and/or bosons, etc. Such problems are of direct interest either in solid state physics, or for cold atoms in optical lattices.

For two-fermion Green's functions ($N_f = 2$), our method is equivalent to that of Ref. [8], but is recast in a simpler form which allows, in 1D, for an analytical solution for any finite-range interaction. More importantly, it has a simple generalization for $N_f > 2$. We study cases with up to $N_f = 5$ and show that these suffice not only to sort out the stability of few-particle bound states, but also to infer the low density phase diagram.

Consider, then, spinless fermions on a 1D chain with $N \rightarrow \infty$ sites, described by the Hamiltonian:

$$\mathcal{H} = -t \sum_i (c_i^\dagger c_{i+1} + h.c.) + U_1 \sum_i n_i n_{i+1} + U_2 \sum_i n_i n_{i+2}$$

where c_i removes a spinless fermion from site i located at $R_i = ia$, and $n_i = c_i^\dagger c_i$. Note that this 1D Hamiltonian is not integrable in the sense of having a Bethe ansatz solution. Because our solution is not linked in any way to such integrability, it can be generalized to higher dimensions, as already mentioned. To illustrate the main idea behind our solution, we discuss in some detail the solution for $N_f = 2$ fermions, after which we generalize to $N_f > 2$. Other possible generalizations, mentioned above, are discussed in the supplementary material [9].

Because the Hamiltonian is invariant to translations, the total momentum of the pair is a good quantum number. As a result, we work with the $N_f = 2$ states:

$$|k, n\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ik(R_i + \frac{n\pi}{2})} c_i^\dagger c_{i+n}^\dagger |0\rangle$$

which describe fermions at a relative distance $n \geq 1$.

We define the two-particle Green's functions:

$$G(m, n; k, \omega) = \langle k, m | \hat{G}(\omega) | k, n \rangle$$

where $\hat{G}(\omega) = [\omega + i\eta - \mathcal{H}]^{-1}$ with $\eta \rightarrow 0_+$ and we set $\hbar = 1$. From the Lehmann representation:

$$G(m, n; k, \omega) = \sum_\alpha \frac{\langle k, m | k, \alpha \rangle \langle k, \alpha | k, n \rangle}{\omega - E_{2,\alpha}(k) + i\eta},$$

where $\{|k, \alpha\rangle\}$ are the two-particle eigenstates with total momentum k , $\mathcal{H}|k, \alpha\rangle = E_{2,\alpha}(k)|k, \alpha\rangle$. Thus, this propagator allows us to find the $N_f = 2$ spectrum and also to get information about its eigenfunctions. Its Fourier transform $G(m, n; k, t) \propto \langle k, m| \exp(-i\mathcal{H}t)|k, n\rangle$ is the amplitude of probability that if initially the two particles (with total momentum k) are at a relative distance na , they will be at a relative distance ma after time t .

Matrix elements of the identity $1 = \hat{G}(\omega)(\omega + i\eta - \mathcal{H})$ lead to $\delta_{n,m} = (\omega + i\eta)G(m, n; k, \omega) - \langle k, m| \hat{G}(\omega)\mathcal{H}|k, n\rangle$. Since $\mathcal{H}|k, n\rangle = U(n)|k, n\rangle - f(k)[|k, n-1\rangle + |k, n+1\rangle]$, where $U(n) = U_1\delta_{n,1} + U_2\delta_{n,2}$ and $f(k) = 2t \cos \frac{ka}{2}$, we get a simple recurrence relation:

$$\delta_{n,m} = [\omega + i\eta - U(n)]G(m, n; k, \omega) + f(k)[G(m, n-1; k, \omega) + G(m, n+1; k, \omega)] \quad (1)$$

This is trivial to solve for an infinite chain if one realizes that for any m of interest, $G(m, n; k, \omega) \rightarrow 0$ as $n \rightarrow \infty$. This is obvious if ω is outside the free two-particle continuum where eigenstates, if any, are bound and therefore wavefunctions decay exponentially with n . It is also true inside the free two-particle continuum. Even though here the wavefunctions are plane-waves, η defines an effective lifetime $\tau \sim 1/\eta$. As such, $G(m, n; k, t) \rightarrow 0$ if na is large compared to the typical distance that particles travel within τ . Thus, the recurrence relation can be solved starting from $G(m, M_c + 1; k, \omega) = 0$ for a sufficiently large cutoff M_c . Of course, the $N_f = 2$ case can be solved analytically exactly (see below). However, the idea can be used for $N_f > 2$ cases, where a numerical solution is needed. Noting that the few-particle Green's functions become arbitrarily small as a “relative distance” M (to be defined below) increases, the recurrence relations can be solved propagating the solution from a cutoff M_c towards small M . M_c is then increased until convergence is reached. The effects of η and M_c on the numerical solution are discussed in the supplementary material.

First, though, we complete the $N_f = 2$ discussion, which has an analytical solution (for details see [9]; we also show there how to deal with a finite-size system in this case). At the Brillouin zone (BZ) edge, since $f(k = \pi/a) = 0$ we find:

$$G(1, n; \frac{\pi}{a}, \omega) = \frac{\delta_{n,1}}{\omega + i\eta - U_1},$$

as expected since $|\frac{\pi}{a}, 1\rangle$ is an eigenstate of \mathcal{H} with energy U_1 . For any $ka \neq \pi$, we find

$$G(1, 1; k, \omega) = \left[\omega + i\eta - U_1 - \frac{[f(k)]^2}{\omega + i\eta - U_2 + z(k, \omega)f(k)} \right]$$

and for any $n \geq 2$,

$$G(1, n; k, \omega) = -\frac{[z(k, \omega)]^{n-1}f(k)G(1, 1; k, \omega)}{\omega + i\eta - U_2 + z(k, \omega)f(k)}.$$

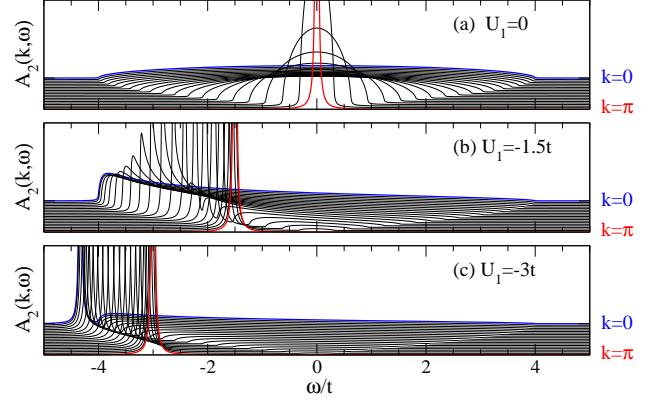


FIG. 1: (color online) $A_2(k, \omega)$ for $U_2 = 0$ and (a) $U_1 = 0$; (b) $U_1 = -1.5t$ and (c) $U_1 = -3t$. As the nn attraction is turned on, a bound state splits from the free two-particle continuum shown in (a). It exists at all momenta if $U_1 < -2t$, but only for large momenta if $U_1 > -2t$. Here $\eta = 0.01$.

Values for $m > 1$ can be obtained similarly. Here, $z(k, \omega)$ is the root of the characteristic equation of this recurrence relation, $(\omega + i\eta) + f(k)(z + \frac{1}{z}) = 0$, for which $|z(k, \omega)| < 1$ [9]. This shows that indeed, $G(1, n; , k, \omega) \rightarrow 0$ as $n \rightarrow \infty$. It is also easy to check that inside the free two-particle continuum, $|\omega| < 2f(k)$, we have $1 - |z(k, \omega)| \sim \eta$, so here G decays exponentially only because $\eta > 0$.

To study the two-particle spectrum, we plot the two-particle spectral weight: $A_2(k, \omega) = -\frac{1}{\pi}\text{Im}G(1, 1; k, \omega)$ in Fig. (1) for $U_2 = 0$, and three values of U_1 . By definition, $A_2(k, \omega)$ is finite at energies in the two-particle spectrum, and its value is related to the probability to find the fermions as nn in that eigenstate. If $U_1 = 0$, $A_2(k, \omega)$ is finite in the free two-particle continuum, ranging from $-4t$ to $4t$ if $k = 0$, while at $k = \pi/a$ only $\omega = 0$ is an eigenstate, hence the δ -function (Lorentzian) seen here. As an attractive U_1 is turned on, the $k = \pi/a$ peak tracks U_1 , and a bound state is pulled below the continuum at nearby k values. For $U_1 > -2t$, this bound state exists only near the BZ edge, while near the Γ point the weak attraction shifts spectral weight to the bottom of the two-particle continuum but is not enough to push a discrete state below it. For $U_1 < -2t$, the bound state becomes the low-energy state at all k . This shows that, for certain ranges of parameters, bound pairs are only stable in some regions of the BZ, which moreover are not necessarily near $k = 0$. It would be interesting to investigate their effects on various response functions.

However, hereafter we focus on the $k = 0$ ground-state (GS). Fig. 2a shows whether in the GS the pair is bound or not, for $U_1 < 0$ and $U_2 > 0$. (Note that such interactions, attractive at short-range and repulsive at longer-range, appear in systems with highly polarizable ions [10]). For $U_1 < -4t$ a bound pair is always stable; even if it had infinite mass, a nn pair of energy U_1 is below the minimum energy of two free fermions,

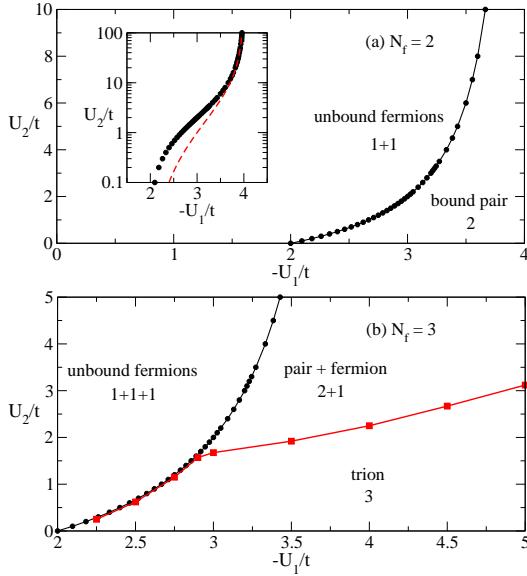


FIG. 2: (color online) Stability diagram for (a) $N_f = 2$, and (b) $N_f = 3$ fermion systems, indicating the nature of the GS. The inset in (a) shows that bound pairs are always stable if $U_1 < -4t$. The dashed line is a perturbational prediction.

of $-4t$. Of course, the kinetic energy of the pair further enhances its stability region. The full line in the inset shows a perturbational estimate for $t \ll |U_1 - U_2|$ [9].

This $N_f = 2$ stability diagram, however, has no predictive power for what happens if more fermions are in the system. For example, if $N_f = 3$, we expect regions where the GS consists of 3 fermions, of a bound pair plus a fermion, or of a bound “trion”. To identify these regions we study $N_f = 3$ Green’s functions, by direct generalization of the $N_f = 2$ approach. Briefly, for any $n_1 \geq 1, n_2 \geq 1$, we define three-particle states:

$$|k, n_1, n_2\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ikR_i} c_{i-n_1}^\dagger c_i^\dagger c_{i+n_2}^\dagger |0\rangle$$

and three-particle Green’s functions:

$$G(m_1, m_2; n_1, n_2; k, \omega) = \langle k, m_1, m_2 | \hat{G}(\omega) | k, n_1, n_2 \rangle.$$

Recurrence relations for these propagators are generated just as for the $N_f = 2$ case. If we define a “relative distance” $M = n_1 + n_2$, hopping of the outside fermions will link Green’s functions with a given M to those with $M \pm 1$. If the central fermion hops, one of the n_1, n_2 values increases by one and the other decreases by one, therefore M remains the same. Thus, the equation of motion links Green’s functions with consecutive $M - 1, M, M + 1$ values, leading to recurrence relations that can be solved in terms of continued fractions of matrices, if we use the insight that propagators vanish as $M \rightarrow \infty$. Generalization to larger N_f values is now straightforward [9].

In higher dimension, we need to combine the “relative distance” with the “Manhattan distance” [11]. For example, in 2D for $N_f = 3$, we associate the plane-wave with

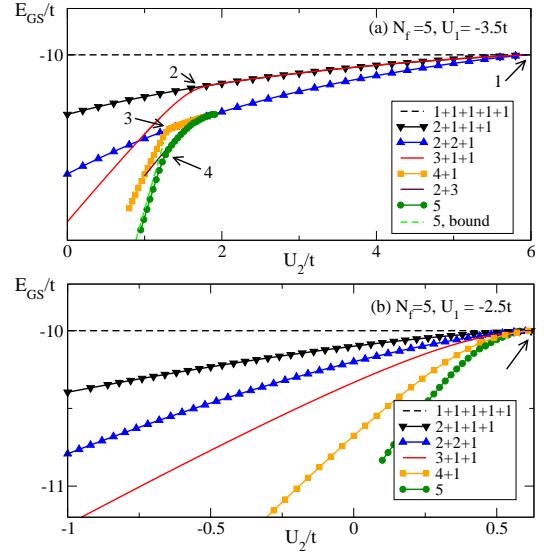


FIG. 3: (color online) $N_f = 5$ GS energy (green circles, label “5”) vs. U_2 for (a) $U_1 = -3.5t$, and (b) $U_1 = -2.5t$. Other lines show the lowest energies of various complexes, and arrows indicate dissociations (see text for details).

the coordinates i_x and i_y of the “central” particle for that axis. The other particles’ coordinates are $i_x - n_{1,x}$, $i_x + n_{2,x}$, respectively $i_y - n_{1,y}$, $i_y + n_{2,y}$, where $n_{i,\alpha} \geq 0$, $i = 1, 2, \alpha = x, y$. If we choose $M = \sum_{i,\alpha} n_{i,\alpha}$ then nn hopping links together only Green’s functions with $M - 1, M, M + 1$. Thus, m particles in 2D is computationally similar to $2m - 1$ particles in 1D. In both cases, $2(m - 1)$ positive integers specify the relative positions, and M is their sum. The key observation is that the equations of motion still group into recurrence relations linking only quantities with $M - 1, M, M + 1$, allowing for an efficient solution (for more details, see [9]).

To study the spectrum of the $N_f = 3$, 1D system, we plot $A_3(k, \omega) = -\frac{1}{\pi} \text{Im}G(1, 1; 1, 1; k, \omega)$. This must have finite spectral weight for $\omega \geq E_{2,GS} - 2t$, corresponding to a continuum of states describing a fermion far away from a pair. (If $E_{2,GS} = -4t$, this continuum starts at $-6t$ and describes 3 free fermions). If the continuum is the lowest spectral feature, then the GS is either a pair+fermion or three fermions, mirroring the $N_f = 2$ situation. However, if a discrete state appears below this continuum, then the GS is a stable bound trion [9]. The stability diagram is plotted in Fig. 2b and shows a region where trions are stable, at large attractive U_1 and weak repulsive U_2 . This is expected since binding a 3rd fermion to a stable pair lowers its energy by roughly $U_1 + U_2$, while a free fermion can lower the total energy by at most $-2t$.

The fact that stable trions are found for $N_f = 3$ does not, however, guarantee that they appear at finite concentrations. Just as the pair+fermion is unstable to trion formation, trions may be unstable to bigger bound complexes, if more particles are present. Indeed, a study of

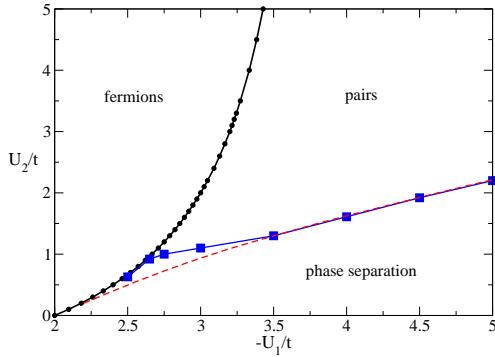


FIG. 4: (color online) Phase diagram at small concentrations. The GS consists either of unbound fermions, or of pairs, or it phase separates into fermion rich and fermion poor regions. The dashed line is an estimate for phase separation (see text).

cases with $N_f = 4$ and 5 fermions proves that trions are actually unstable. This is shown in Fig. 5(a) where we plot the energy of the $N_f = 5$ GS vs. U_2 (line marked “5”) at $U_1 = -3.5t$. The other lines show energies where a continuum could appear, *e.g.* $E_{2+2+1} = 2E_{2,GS} - 2t$ is the lowest energy of two pairs plus a fermion, $E_{2+3} = E_{2,GS} + E_{3,GS}$ is the lowest energy for a pair plus a trion, etc. The arrows indicate various dissociations. Arrow 1 shows when a pair becomes more stable than 2 fermions ($E_{2+1+1+1} < E_{1+1+1+1+1}$), while arrow 2 shows when a trion becomes more stable than a pair+fermion ($E_{3+1+1} < E_{2+1+1+1}$), see Figs. 2a,b. A trion+fermion is unstable to either two pairs (at larger U_2) or a 4-fermion bound complex (smaller U_2). The boundary between the two is marked by arrow 3 ($E_{4+1} = E_{2+2+1}$). But 4-fermion bound states are not stable either, since $E_{4+1} < \min(E_{2+3}, E_5)$ (arrow 4 marks where the 5-fermion bound complex breaks into a pair+trion). Below it, E_5 is indeed in good agreement with the perturbational estimate for the energy of a 5-bound complex $E_{5,B} = 4U_1 + 3U_2 + 2t^2/(U_1 + t^2/U_1 - 2t^2/(U_1 + U_2))$, shown by the dashed line indexed “5, bound”.

What happens as N_f increases becomes clear if we realize that arrows 3 and 4 point to essentially the same U_2 value. If more fermions are added, below this U_2 we expect a bigger and bigger bound complex – in other words, phase separation occurs and the system splits into a fermion rich and a fermion poor region. Above this, a gas of pairs is stable (plus one trion, if N_f is odd). That this inference is correct is verified by the following argument. This critical value should be given by the condition that adding two more particles to a fermion rich region (which changes energy by about $2U_1 + 2U_2$, because of extra interactions) should be energetically favorable to having a bound pair far away. From $2U_2 + 2U_1 < E_{2,GS}$ we find $U_2 = 1.29t$ if $U_1 = -3.5t$, in good agreement with the value $U_2 = 1.3t$ pointed to by arrows 3 and 4.

Thus, based on these few-particles results, we can infer

the phase diagram of this model at small concentrations, shown in Fig. 6. The dashed line shows the estimate discussed above, accurate for large U_1, U_2 (at smaller U_1 , t comes into play since the extra fermions need not be fully localized at the edge of the fermion rich region). If $U_1 > -2.6t$, the transition is from phase separation to unbound fermions as U_2 increases. This is shown, for $U_1 = -2.5t$, in Fig. 5b: here each bigger complex is more stable than any smaller ones, if $U_2 < 0.63t$ (arrow).

While we are not aware of numerical studies of this model, the good agreement with various asymptotic estimates as well as with known results for spin- $\frac{1}{2}$ Hamiltonians [9], supports the accuracy of our results. This work shows that even such a simple model has a rich behavior that can be uncovered with this method.

To summarize, we have shown how to calculate few-particle Green’s functions on an infinite 1D chain. The information obtained from them sheds light on the stability of few-particle bound states. It also illustrates the dangers of an insufficient analysis – if we stopped at $N_f = 3$, we would conclude that trions are stable in a large region of the parameter space, in this model. Analysis for larger N_f shows that addition of more particles leads to instability of trions, and furthermore allows us to find the phase diagram for small concentrations.

Although these results are for a 1D model, as discussed above this method generalizes to higher-D if the hopping is nearest-neighbor only. This opens the way to study the stability of trions and bi-excitons in realistic lattice models. Such work is currently under way.

Acknowledgments: I thank I. Affleck, G. Sawatzky, P. Stamp, F. Zhou and S. Yarlagadda for useful discussions. This work was supported by NSERC and CIFAR.

-
- [1] X.-J. Liu, H. Hu, and P. D. Drummond, Phys. Rev. Lett. **102**, 160401 (2009); Phys. Rev. A **82**, 023619 (2010); Phys. Rev. B **82**, 054524 (2010).
 - [2] V. Efimov, Phys. Lett. B **33**, 563 (1970); Sov. J. Nucl. Phys. **12**, 589 (1971); JETP Lett. **16**, 34 (1972).
 - [3] for example, see S. E. Pollack, D. Dries and R. G. Hulet, Science **326**, 1683 (2009).
 - [4] for example, see D. MacNeill and F. Zhou, Phys. Rev. Lett. **106**, 145301 (2011).
 - [5] F. J. Teran *et al.*, Phys. Rev. B **71**, 161309(R) (2005)
 - [6] R. Matsunaga, K. Matsuda, and Y. Kanemitsu, Phys. Rev. Lett. **106**, 037404 (2011).
 - [7] T. F. Ronnow, T. G. Pedersen and H. D. Cornean, Phys. Rev. B **81**, 205446 (2010).
 - [8] G. A. Sawatzky, Phys. Rev. Lett. **39**, 504 (1977);
 - [9] Supplementary Material is appended at the end of this document.
 - [10] M. Berciu, I. Elfimov and G. A. Sawatzky, Phys. Rev. B **79**, 214507 (2009).
 - [11] M. Berciu and A. Cook, Europhys. Lett. **92**, 40003 (2010).

SUPPORTING MATERIAL

Further support for this phase diagram

As discussed in the main text, the phase diagram we derived from the few-particle Green's functions is supported by the asymptotic lines shown in Figs. 2a (inset) and Fig. 4. We are not aware of any numerical studies of this model that could be used for direct comparison, although it bears mentioning that once M_c is large enough that convergence has been achieved (see discussion and examples below), these results are exact – there is no approximation involved in obtaining them.

However, additional support for these results can be obtained from studies of spin- $\frac{1}{2}$ Hamiltonians. Through a Jordan-Wigner transformation [1], the Hamiltonian for spinless fermions studied here can be mapped into:

$$\mathcal{H} = \sum_i [-2t(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + U_1 S_i^z S_{i+1}^z + U_2 S_i^z S_{i+2}^z].$$

The case $U_1 < 0, U_2 > 0$ corresponds to ferromagnetic nearest-neighbour Ising interaction and frustrating anti-ferromagnetic next nearest-neighbour Ising interaction.

For $U_2 = 0$, the phase diagram of this model is well-known: it consists of a ferromagnet for $|U_1| > 2t$ and a Luttinger liquid otherwise [2]. The ferromagnet corresponds to phase-separation in the fermion language, since the magnetization is linked to the density of fermions. The unpaired fermions phase is reasonably linked to the Luttinger liquid, so this line of the phase diagram agrees with other known results.

While we could not find a study of the spin model with $U_2 \neq 0$, it is expected that an increase in U_2 frustrates the ferromagnetic phase and eventually makes it unstable. We believe that the pairs phase is a charge 2 Luttinger liquid, a sort of 1D version of a p-wave superconductor. Such phases are fairly well known [2, 3].

Details for the $N_f = 2$ solution

As discussed, because the Hamiltonian is invariant to translations it is convenient to use the two-fermion states:

$$|k, n\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ik(R_i + \frac{n\alpha}{2})} c_i^\dagger c_{i+n}^\dagger |0\rangle.$$

The method can be trivially extended to systems with disorder because using these translational states is not an essential ingredient of the method.

For a finite-size chain with N sites, in order to not double count the states, we must restrict $1 \leq n \leq N_{max}$, where $N_{max} = \frac{N}{2}$ if N is even, respectively $N_{max} = \frac{N+1}{2}$ if N is odd. In other words, when considering the two fermions on the closed ring, we take the distance between

them to be the shortest possible “arc”, $n \equiv \min(n, N-n)$. Using $e^{ikNa} = 1$, it follows that for any $1 \leq n \leq N_{max}$

$$|k, N-n\rangle = -e^{ik\frac{Na}{2}} |k, n\rangle.$$

The equations of motion for the two-particle Green's functions were derived in the main text. For $m = 1$, and using the notation $G(1, n; k, \omega) \rightarrow a_n$, they are:

$$(\omega + i\eta - U_1)a_1 + f(k)a_2 = 1 \quad (2)$$

$$(\omega + i\eta - U_2)a_2 + f(k)(a_1 + a_3) = 0 \quad (3)$$

$$(\omega + i\eta)a_n + f(k)(a_{n-1} + a_{n+1}) = 0 \quad (4)$$

for $3 \leq n < N_{max}$, and finally

$$(\omega + i\eta)a_{N_{max}} + f(k) \left[1 - e^{-ika\frac{Na}{2}} \right] a_{N_{max}-1} = 0 \quad (5)$$

A numerical solution is now trivial.

However, we can do better. First, note that for $ka = \pi$ we have $f(k) = 0$, and so the solution is:

$$G(1, n; \frac{\pi}{a}, \omega) = \frac{\delta_{n,1}}{\omega + i\eta - U_1}.$$

This is expected, since $|\frac{\pi}{a}, 1\rangle$ is an eigenstate of the full Hamiltonian with energy U_1 , as can be easily checked.

For any $ka \neq \pi$, the equations for $3 \leq n \leq N_{max} - 1$ can be solved analytically. Their general solution is:

$$a_n = \alpha z^n + \frac{\beta}{z^n}$$

where z and z^{-1} are the roots of the characteristic equation: $(\omega + i\eta) + f(k)(z + \frac{1}{z}) = 0$. We choose $z \equiv z(k, \omega)$ to be the root for which $|z| < 1$. This is always uniquely defined for any $\eta > 0$, since the product of the two roots

$$z_\pm = \frac{1}{2} \left[-\frac{\omega + i\eta}{f(k)} \pm \sqrt{\left(\frac{\omega + i\eta}{f(k)} \right)^2 - 4} \right]$$

is 1. The solution is now immediate. The last equation for $n = N_{max}$ fixes the ratio of β/α , the solution is then propagated down to $n = 2$, and one uses the first two equations to find a_1 and α , completing the solution.

These results have a very straightforward physical interpretation. Note that the general recurrence equation for $3 \leq n \leq N_{max}$ is the same that describes *two free fermions*. For a given k , the two-fermion continuum spans the energies $\{\epsilon_{k-q} + \epsilon_q\}_q = [-4t \cos \frac{ka}{2}, 4t \cos \frac{ka}{2}]$, where $\epsilon_k = -2t \cos(ka)$ is the free particle energy.

This explains why for energies outside this range $|\omega| \geq 2f(k) = 4t \cos \frac{ka}{2}$, we find the two roots $z, 1/z$ to be real (when $\eta \rightarrow 0$), and such that $|z| \rightarrow 0$ as $|\omega| \rightarrow \infty$. This shows that here the two-particle Green's function decays exponentially with n , as expected since there are no free two-particles eigenstates at these energies. The exponentially increasing $\frac{\beta}{z^n} \sim z^{N-n}$ part is a finite size

effect: on a finite chain, the inter-particle distance eventually decreases as $n \rightarrow N$. In the limit $N \rightarrow \infty$, this contribution must vanish, in other words in the thermodynamic limit we must have $a_n = za_{n-1} = \alpha z^n$ as a purely exponentially decreasing function with distance. This is consistent with the fact that the solution must be insensitive to how we end the recurrence relation (what is the boundary condition) as $N \rightarrow \infty$.

For certain values of U_1, U_2 , new eigenstates may appear outside the free two-particle continuum. These describe bound pairs, therefore we expect their wavefunctions (and the associated Green's functions) to decay exponentially with the distance n between the particles. This is fully consistent with the previous discussion. In particular, since $|z| \rightarrow 0$ as $\omega \rightarrow -\infty$, it follows that lower-energy pairs are more tightly bound.

On the other hand, inside the free two-particle continuum, $|\omega| < 2f(k)$, we find $|z| \rightarrow 1$ as $\eta \rightarrow 0$. As a result, the two contributions to a_n become oscillatory functions, underlying the fact that there are freely propagating two-particle eigenstates at these energies. The interaction will be responsible for scattering leading to phase-shifts, however at these energies the two particles can propagate arbitrarily far from each other, if $\eta = 0$.

Using a finite η (which we are forced to do, for numerical reasons), results in $1 - |z| \sim \eta$, in other words there is slow exponential decay at these energies as well, but now controlled by η . Physically, this is because the finite η introduces a “life-time” for these particles. As a result, if the distances $n, N - n$ are very large compared to the typical relative distance the two free particles can explore in their lifetime $\tau \sim \frac{1}{\eta}$, the probability for the pair to be

at such distances decreases exponentially, and so do the Green's functions. It follows that in the thermodynamic limit, we can again take $a_n = \alpha z^n$. Then, the solution in the thermodynamic limit is trivial since we only need to solve the equations for a_1 and a_2 using $a_3 = z(k, \omega)a_2$. The solution is listed in the main text. Generalization to longer (but finite) range interactions is trivial, as is finding the solution for other m values.

$N_f = 3$ in the thermodynamic limit

Based on the arguments discussed above, in the limit of an infinite chain we expect the Green's functions to decay exponentially at all energies, with an exponent controlled by η inside the three-particle continuum, and by the inverse of the distance between ω and the continuum's band-edge, for energies outside the continuum.

We use three-particle states of total momentum k :

$$|k, n_1, n_2\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ikR_i} c_{i-n_1}^\dagger c_i^\dagger c_{i+n_2}^\dagger |0\rangle$$

where $n_1 \geq 1, n_2 \geq 1$. Since we take $N \rightarrow \infty$, the states with $n_1 \sim N_{max}, n_2 \sim N_{max}$ become irrelevant and we do not need to worry about properly counting them; because of the finite lifetime, even inside the continuum particles cannot travel that far from each other. For a finite chain, however, proper counting is important (see below).

The equations of motion for the three-particle Green's functions defined in the main text, are:

$$\begin{aligned} \delta_{n_1, m_1} \delta_{n_2, m_2} &= (\omega + i\eta - U_{n_1, n_2}) G(m_1, m_2; n_1, n_2; k, \omega) \\ &+ t [G(m_1, m_2; n_1 - 1, n_2; k, \omega) + G(m_1, m_2; n_1 + 1, n_2; k, \omega) \\ &+ e^{ika} G(m_1, m_2; n_1 - 1, n_2 + 1; k, \omega) + e^{-ika} G(m_1, m_2; n_1 + 1, n_2 - 1; k, \omega) \\ &+ G(m_1, m_2; n_1, n_2 + 1; k, \omega) + G(m_1, m_2; n_1, n_2 - 1; k, \omega)]. \end{aligned}$$

Here, $U_{n_1, n_2} = U_1(\delta_{n_1, 1} + \delta_{n_2, 1}) + U_2(\delta_{n_1, 2} + \delta_{n_2, 2} + \delta_{n_1+n_2, 2})$ is the interaction energy when the three particles are at relative distances n_1, n_2 from each other. The remaining terms describe the effect of hopping on the $|k, n_1, n_2\rangle$ state. The first two terms come from the hopping of the left-most particle, which changes n_1 . The next two terms come from the hopping of the central particle, which keeps $n_1 + n_2$ constant, and the last two terms are from the hopping of the rightmost particle, which changes n_2 . If $n_1 = 1$ then $G(m_1, m_2; n_1 - 1, n_2, k, \omega) \equiv 0$ since this hopping process is not allowed for spinless fermions, and similarly for n_2 . For $N \rightarrow \infty$ we need not worry what

happens as $n_1, n_2 \sim N_{max}$, since the Green's functions vanish before the particles go so far from each other.

Suppose we are interested in $m_1 = m_2 = 1$ and use the shorthand notation $a(n_1, n_2) = G(1, 1; n_1, n_2; k, \omega)$. The resulting infinite (in the thermodynamic limit) system of coupled recurrence relations can be solved as follows. We define the vectors

$$V_M = \begin{pmatrix} a(1, M-1) \\ a(2, M-2) \\ \vdots \\ a(M-1, 1) \end{pmatrix}$$

which collect all the Green's functions with the same “rel-

“relative distance” $M = n_1 + n_2$. Its dimension is $M - 1$, although for special values of k there are further symmetries that can lower it. For example, at $k = 0$ we have $a(n, M - n) = a(M - n, n)$ and the dimension is halved.

The special property of Hamiltonians with only nearest-neighbor hopping is that the resulting equations of motion only link three vectors with consecutive relative distances. In other words, for any $M \geq 3$, we can recast the recurrence equations as:

$$\gamma_M V_M = \alpha_M V_{M-1} + \beta_M V_{M+1} \quad (6)$$

where $\alpha_M, \beta_M, \gamma_M$ are very sparse matrices whose matrix elements are simple functions of k, ω that can easily be read off the equations of motion. Because we know that all Green’s functions must vanish in the limit $M \rightarrow \infty$, the solution of this recurrence equation is given by:

$$V_M = A_M V_{M-1}$$

where the matrices A_M are given by continued fractions:

$$A_M = [\gamma_M - \beta_M A_{M+1}]^{-1} \alpha_M$$

and can be calculated starting with $A_{M_c+1} = 0$ at a sufficiently large cutoff M_c .

Once all these matrices are known, and in particular A_3 which links $a(1, 2)$ and $a(2, 1)$ to $a(1, 1)$, we can use the equation of motion with $n_1 = n_2 = 1$ to find:

$$G(1, 1; 1, 1; k, \omega) = \frac{1}{\omega + i\eta - 2U_1 - U_2 + t[A_3]_{1,1} + A_3[2,1]},$$

from which we can then get all the other propagators.

To illustrate the effect of the numerical parameters η and M_c , we analyze the three-particle spectral weight:

$$A_3(\omega) = -\frac{1}{\pi} \text{Im}G(1, 1; 1, 1; k=0, \omega) \quad (7)$$

This is finite for all energies ω in the $k = 0$, $N_f = 3$ spectrum, and its weight gives the probability of having the three fermions located on three consecutive sites.

Just like for $N_f = 2$, whether a bound trion is the ground-state or not is determined by whether a discrete Lorentzian appears below the continuum, or not. The continuum starts at $E_{2,GS} - 2t$, where $E_{2,GS}$ is the GS energy of the $N_f = 2$ case. If the parameters are such that bound pairs are not stable, then $E_{2,GS} = -4t$ and the three-particle continuum starts at $-6t$. However, if a bound pair is stable, then the continuum moves to lower energies, and consists of states where a free particle scatters off a bound pair (other higher-energy features are also present, but not of interest for our analysis).

In Fig. (5), we show $A_3(\omega)$ for $U_1 = -3t, U_2 = 0$ and three sets of parameters η, N_c . The dashed vertical line shows the expected on-set of the continuum, at $E_{2,GS} - 2t$ [for these parameters, $E_{2,GS} \approx -4.33t$, see Fig. 1c in the main text]. Clearly, $A_3(\omega)$ shows a continuum starting

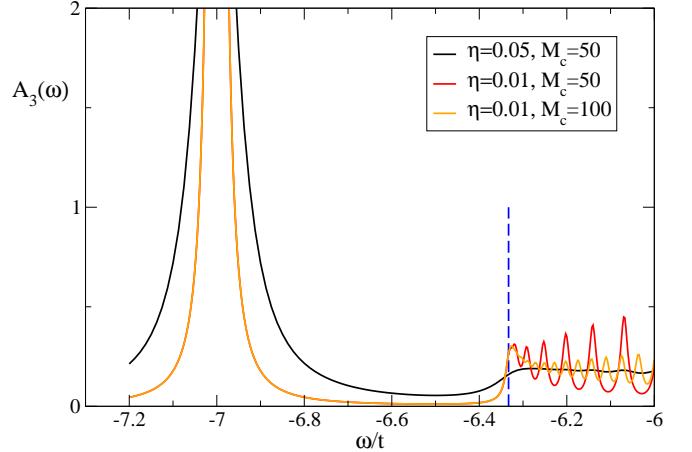


FIG. 5: $A_3(\omega)$ vs ω for $U_1 = -3t, U_2 = 0$, for various values of the broadening η and the cutoff M_c . The dashed line shows the expected continuum onset at $E_{2,GS} - 2t$.

at this energy, but there is also a Lorentzian peak below it, indicating a stable trion for these parameters.

Note that the spectral weight in the continuum depends on the specific broadening η and cutoff M_c used. This dependence can be understood easily. M_c is the cut-off at which we set the Green’s functions to zero. Physically, this is equivalent with adding an effective “interaction” which becomes infinite if the total relative distance between particles $n + m > M_c$, and is zero otherwise. As is the case for any system in a “box”, we expect the continuum to be replaced by a set of discrete levels, with a spacing $\delta E \sim 1/M_c$. These states, however, are broadened by η . This explains why the first curve is much smoother than the second one, even though they have the same M_c . On the other hand, the third curve has M_c increased by a factor of two, and indeed there are roughly twice as many oscillations marking the discrete peaks. For any value of M_c , the curve becomes smooth if η is large enough so that $\delta E \sim \eta$. As already discussed, physically this means that the lifetime $\tau \sim 1/\eta$ is so short that the particles cannot travel up to the boundaries of this potential “box” defined by M_c .

Below the continuum, the spectral weight is insensitive to M_c , because the states that appear here (if any) are bound well inside this “box”. The broadening η is still reflected in the shape of the Lorentzian: although not shown entirely in Fig. 5, the peak for the smaller η is 5 times narrower and taller, as expected. This insensitivity to M_c is very convenient, because it means that one can get very good estimates for the energy of strongly bound states using rather small M_c values. Of course, if the binding energy is very small, then one has to increase M_c until convergence is achieved.

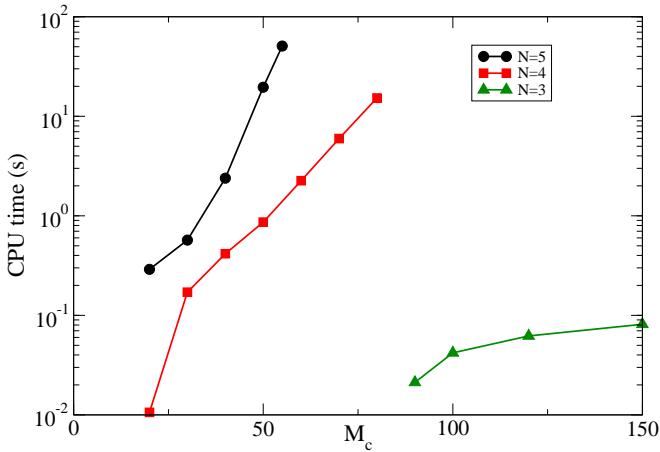


FIG. 6: CPU time for one frequency, vs. cutoff M_c , for systems with $N_f = 3, 4, 5$.

Higher N_f in the thermodynamic limit

It should now be apparent that the method generalizes straightforwardly to any case with an odd number N_f of particles. We choose the reference location i as being that of the central particle, and index states in terms of the absolute values of the relative distances of all other particles $n_1, n_2, \dots, n_{N_f-1}$ with respect to the central particle. In the equation of motion, hopping of any of these other particles will increase or decrease its own n_i by 1, so the “relative distance” $M = \sum_{i=1}^{N_f-1} n_i$ varies by 1. If the central particle hops to the right, for example, this increases by 1 all the distances to all particles to its left, and decrease by 1 all distances to all particles to its right. Since there are equal numbers of particles to the left and to the right of the central particle, then M is unchanged.

For an even N_f , we choose as the reference particle either of the two central particles. In this case, the “relative distance” is changed by 1 when any of the particles hop, including the “central” one.

In either case, the recurrence equation can still be cast in the general form of Eq. (6) and can be solved by similar means. Of course, the larger N_f is, the larger is the dimension of V_M , so eventually one runs out of computational power to calculate the continued fractions numerically. This is the factor that limits what values of N_f can be considered.

Fig. 6 gives the real time to calculate the spectral weight at one frequency on a 4-core CPU, for systems with $N_f = 3, 4$ and 5 fermions. As expected, the run times increase quite fast with both N_f and the chosen cutoff M_c . Note that for $N_f = 3, 4$ we showed data for M_c much larger than what is needed to achieve convergence, simply because for smaller values the CPU time becomes independent of M_c , showing that it is determined by other tasks, not by the computation of the con-

tinued fractions which is the most time-consuming part at large M_c . In fact, $M_c = 50$ sufficed to achieve convergence even in the most delicate cases discussed in the main article, namely where a bound state is very close to a continuum (*i.e.* near a dissociation process). As already mentioned, here one needs to use a small η and therefore a larger M_c to be able to separate such close-by features. If the energy of the bound complex is well below the continuum, on the other hand, much smaller M_c suffices and calculations are much faster.

In practice, it is useful to first use a fairly small M_c to quickly scan a large range of energies to see where the main features are. Of course, one particularly useful characteristic of this calculation is that the spectrum for a given number N_f of fermions must have one or more continua at energies determined by the spectra with fewer fermions, which are known. This gives not only a chance to validate the computation, but also a very useful indication of where features are expected in the spectral weight. If a N_f -bound complex is stable, its corresponding Lorentz peak is below the lowest-energy continuum and must be found by searching for a peak in the spectral weight in the infinite range of energies lying below this lowest continuum. Even in this case, one may use perturbation theory as a first guide to where the peak may be. As an example, see line “5, bound” in Fig. 3a which provides an estimate for the energy of the 5-fermion bound complex. To zero order, its energy is $E_{5,B} = 4U_1 + 3U_2$, since a configuration with 5 fermions occupying consecutive sites has 4 nn and 3 nnn pairs. If U_1, U_2 are comparable to t , then one can use perturbation to allow the end fermions to hop one site on and off the end of the complex; this further lowers the energy by $2t^2/U_1$ (note that $U_1 < 0$), since the resulting configuration only has 3 nn and 3 nnn pairs. If needed, 2nd and higher order corrections can be obtained by including further possible configurations, in a standard fashion. Using such guidance plus low- M_c scan of a large range of energies, the rough position of the peak can be found efficiently, after which M_c is increased until the energy of the peak is converged to the desired precision. Note that since this peak is a Lorentzian with a known broadening η , as few as 2 points close to its maximum suffice to extract its maximum and its weight from fitting.

This is why even though for $N_f = 5$ and $M_c = 50$ it takes ~ 20 s to calculate the spectral weight at one frequency, one can actually identify the GS energy with high precision within very few minutes, for a given value of the parameters. This is also why we are confident that this type of calculation can be successfully extended to larger N_f , especially if clusters with more than 4 CPUs are used to further speed up the computation. We stopped at $N_f = 5$ here simply because this value was sufficient to deduce the phase diagram for this model.

Mix of two different kinds of fermions

We now briefly discuss the generalization to a mix of two different types of spinless fermions, still on a 1D infinite chain. Let c_i and d_i be their corresponding annihilation operators. For spin- $\frac{1}{2}$ fermions, one can take $a_{i,\uparrow} \equiv c_i; a_{i,\downarrow} \equiv d_i$. The model Hamiltonian we consider is a direct generalization that used in the main text:

$$\begin{aligned} \mathcal{H} = & -t_c \sum_i (c_i^\dagger c_{i+1} + h.c.) + U_{1,c} \sum_i n_{c,i} n_{c,i+1} + U_{2,c} \sum_i n_{c,i} n_{c,i+2} \\ & - t_d \sum_i (d_i^\dagger d_{i+1} + h.c.) + U_{1,d} \sum_i n_{d,i} n_{d,i+1} + U_{2,d} \sum_i n_{d,i} n_{d,i+2} \\ & + U_0 \sum_i n_{c,i} n_{d,i} + U_{1,m} \sum_i (n_{d,i} n_{c,i+1} + h.c.) + U_{2,m} \sum_i (n_{d,i} n_{c,i+2} + h.c.). \end{aligned} \quad (8)$$

In other words, each species has both nn and nnn interactions, while the mixed interactions are on-site, nn and nnn. Of course, if the two spinless fermions correspond to different spin-projections of the same spinful fermion, and the interactions are spin-independent, then one expects $U_{1,c} = U_{1,d} = U_{1,m}$ etc.

Consider first a mixed pair with a total momentum k . One expects to be able to factorize the two-particle states into analogs of “singlet” and “triplet” (with $m = 0$) states, which should not mix with one another through hopping, so that each should have its own set of recurrence relations. This is indeed true, however at finite momentum these symmetries get mixed and identifying

the proper states requires a bit of work. The solution is as follows. We define:

$$t(k) = t_c e^{ik\frac{ka}{2}} + t_d e^{-ik\frac{ka}{2}} = T(k) e^{i\phi_k}$$

where $T(k) = \sqrt{t_c^2 + t_d^2 + 2t_c t_d \cos(ka)}$ and $\cos \phi_k = (t_c + t_d) \cos \frac{ka}{2} / T(k)$. Then, let:

$$|k, s, 0\rangle = \frac{1}{\sqrt{N}} \sum_i e^{ikR_i} c_i^\dagger d_i^\dagger |0\rangle$$

and for any $n \geq 1$,

$$|k, s, n\rangle = \frac{1}{\sqrt{2N}} \sum_i e^{ikR_i + \frac{na}{2}} (e^{in\phi_k} c_i^\dagger d_{i+n}^\dagger - e^{-in\phi_k} d_i^\dagger c_{i+n}^\dagger) |0\rangle \quad (9)$$

$$|k, t, n\rangle = \frac{1}{\sqrt{2N}} \sum_i e^{ikR_i + \frac{na}{2}} (e^{in\phi_k} c_i^\dagger d_{i+n}^\dagger + e^{-in\phi_k} d_i^\dagger c_{i+n}^\dagger) |0\rangle \quad (10)$$

The “s” and “t” labels are because at $k = 0$, and if these are spin-up and spin-down fermions, these states describe the usual singlet and triplet combinations.

It is now easy to check that the recurrence relations do not mix “s” and “t” states together, and each set can be solved similarly to that for the spinless $N_f = 2$ case. This is a double bonus. First, because it keeps the recurrence equations simpler, which makes the calculation more efficient. More importantly, one can figure out the symmetry of the bound states that form, based on which Green’s functions exhibit poles at those energies.

More mixed fermions

Generalization to more particles follows closely. The main ingredient, namely that a relative distance can be defined, and that hopping only varies it by at most 1, stays the same. The complication is that now particles of unlike type can pass by each other, so for example for a three-particle calculation with relative distance $M = n + m$, one generally has to include all states like $\sum_i e^{ikR_i} c_{i-n}^\dagger c_i^\dagger d_{i+m}^\dagger |0\rangle$, $\sum_i e^{ikR_i} c_{i-n}^\dagger d_i^\dagger c_{i+m}^\dagger |0\rangle$ and $\sum_i e^{ikR_i} d_{i-n}^\dagger c_i^\dagger c_{i+m}^\dagger |0\rangle$. Thus, the dimension of the vectors with a given relative distance is bigger than if the particles were identical. Again, careful consideration of symmetries (especially at $k = 0$) lowers the dimension and make the calculation more efficient, besides provid-

ing information on the symmetry of the bound states.

Bosons

The calculation can be carried over to bosons trivially. The main difference is that one can place any number of bosons on the same site, so there are additional recurrence equations describing states with shorter relative distances than possible for fermions. The nn hopping insures the same general structure of the recurrence equations, and in fact for the terms where there are no multiple bosons at the same site, the equations are identical with those for fermions in similar configurations.

Higher dimensions

To obtain this, one has to combine together the idea of a “relative distance”, described above for multiple particles, with that of a “Manhattan distance” which we introduced in Ref. 4 to show how to calculate single-particle Green’s functions in higher dimensions. For example, for two particles on a 2D square lattice, one needs two integers $\mathbf{n} = (n_x, n_y)$ to characterize the relative distance between the two particles in states of the form $|\mathbf{k}, \mathbf{n}\rangle \sim \sum_{i_x, i_y} e^{i\mathbf{k} \cdot \mathbf{R}_i} c_i^\dagger c_{i+\mathbf{n}}^\dagger |0\rangle$. Some restrictions apply to the allowed values of n_x, n_y so that double counting is avoided. For example, we can choose $n_x \geq 0$; if $n_x = 0$ then only $n_y \geq 0$ is needed, while if $n_x > 0$, n_y can take both positive and negative values [5]. Nearest neighbor hopping will link the Green’s function for this ket to the ones corresponding to kets with $(n_x \pm 1, n_y)$ and $(n_x, n_y \pm 1)$. As a result, here we should choose $M = |n_x| + |n_y|$ as a sum of the relative distances projected along all the axes – this is a “Manhattan distance” characterizing the relative distance between the two particles in this state. Nearest-neighbor hopping then preserves the general structure of linking Green’s functions with a given M to only others with $M \pm 1$, and the general approach of rewriting the equations of motions in terms of continued fractions carries over. In fact, this problem is very similar in structure to that of 3 fermions in 1D, where we also need two integers n_1, n_2 to characterize each internal arrangement, and where $M = n_1 + n_2$. The main difference is that in 2D, n_y could be negative as well, in other words there are roughly twice as many states with a given M then for the 3 particles in 1D. This suggests a corresponding increase in the computational time. In reality, even this increase can be eliminated, if one explicitly works with pairs of *s*-wave or *d*-wave symmetry. In the former case, the Green’s functions corresponding to a given n_x and $\pm n_y$ are equal, while in the latter case, they have equal magnitude but opposite sign. In either case, the actual number of unknowns is halved. As a result, the 2D calculation for either an *s*-wave or *d*-

wave pair is basically equivalent to a 1D calculation for 3 particles.

The generalization to 3 particles is described briefly in the main article. In this case, we need 4 integers to describe the relative positioning with respect to the “central” particle (note that different particles can play this role, for different axes). In 1D, 4 integers are needed to describe the relative arrangements of 5 particles. In general, m particles in 2D require $2(m - 1)$ integers to specify relative positioning from a “central” particle, and as such, this calculation maps onto a calculation with $2m - 1$ particles in 1D. Just as discussed above for $m = 2$, at first sight there are more states with the same total M in the 2D problem then in the 1D one, because some of the 2D integers could be negative while the 1D ones are all positive. However, if symmetries are properly enforced this overall multiplication factor can be removed, at least at $k = 0$. As a result, one finds not only the spectrum but also the symmetry of the bound complex (if, indeed, such a bound complex is stable).

This is why in terms of running times for higher-D, a reasonable estimate can be obtained based on running times in 1D. For example, the 2D, $N_f = 2$ case discussed above is roughly equivalent to a 1D, $N_f = 3$ computation, since in both cases the configurations are characterized by 2 integers. It follows that stability for trions ($N_f = 3$) and bi-excitons ($N_f = 4$) can be studied very easily in 2D, since it involves problems similar to $N_f = 5$, respectively $N_f = 7$ in 1D. In 3D, study of trions would be equivalent to investigating $N_f = 7$ in 1D, which can certainly be accomplished in a reasonable time on a regular desktop with a 4-core CPU. To study bi-excitons in 3D (equivalent to $N_f = 10$ in 1D), it may be needed to use a bigger cluster to lower the computation time. Of course, if the bound complex is stable, this will be confirmed by a small M_c run, in an efficient fashion.

Longer-range hopping and/or finite chains

In these cases, it is impossible to recast the equations of motion in terms of recurrence equations for consecutive vectors V_{M-1}, V_M, V_{M+1} . For longer range hopping, this is because the relative distance will be changed by at least ± 2 for second-nearest neighbor hopping. Even for nearest-neighbor only hopping, in a finite system this simple rule is broken for states with particles separated by maximum allowed distances. The only exception is for $N = 2$ on a chain, where as discussed, the hopping from $n = N_{max}$ to $N_{max} + 1$ is actually mapped into hopping to $N_{max} - 1$, up to a phase factor. In all other cases, the hopping out of these states with maximally allowed relative distances will map into states which can have quite different M values.

One may still obtain a solution for such cases, by solving all of them together as a linear system, instead of

factorizing them into a recursive set based on their M values. While the dimension of this linear system is much bigger, the matrix is extremely sparse and can be dealt with efficiently by various known algorithms.

For an infinite system with longer range hopping, if one is interested in bound states, then one can set a quite small cutoff resulting in a reasonable computational task. For a finite-size chain, one needs some physical intuition to decide what states (Green's functions) can be removed from the calculation, i.e. how to define a “cutoff”. We are currently investigating such problems.

-
- [1] P. Jordan and E. Wigner, Z. Phys **47**, 631 (1928).
 - [2] T. Giamarchi, “*Quantum Physics in One Dimension*”, (Clarendon Press, 2005).
 - [3] H. J. Schulz, Phys. Rev. B **34**, 6372 (1986).
 - [4] M. Berciu and A. M. Cook, EuroPhys. Lett. **92**, 40003 (2010).
 - [5] for a similar discussion, see M. Berciu and G. A. Sawatzky, Phys. Rev. B **79**, 214507 (2009).